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14. ABSTRACT
This project is concerned with the development of a precision measurement technique for determining the complex dielectric constant (or permittivity) of biological molecules in liquids at frequencies below 300 GHz. The development of precise measuring techniques is critical for advancing understanding of the interaction between biological molecules and terahertz (THz) frequency electromagnetic fields.
Waveguide cavities have been used to obtain the permittivity of liquids by measurement of the lowest order

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Submillimeter-wave Resonators for Investigation of the Dynamical Properties of Biological Molecules

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This project is concerned with the development of a precision measurement technique for determining the complex dielectric constant (or permittivity) of biological molecules in liquids at frequencies below 300 GHz. The development of precise measuring techniques is critical for advancing understanding of the interaction between biological molecules and terahertz (THz) frequency electromagnetic fields. Waveguide cavities have been used to obtain the permittivity of liquids by measurement of the lowest order resonant mode, guaranteeing single-moded operation and thus ease of modeling from fundamental principles. However, due to cavity size scaling with frequency, measurements with the fundamental mode have been limited to below 50 GHz. Recent work has instead investigated the rigorous modeling of over-moded cavities. By the ability to keep the cavity large and easily machineable, such an approach would enable the use of a resonator for acquisition of high precision measurements at higher frequencies. This is the method adopted by this project, and developed for the measurement of liquids. A preliminary measurement setup was created and tested, then used a guide for a new measurement setup. Concurrently the modeling was developed, starting from a closed resonator to the more accurate, yet complex, four-port junction.

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Angelique Sklavounos	1.00	
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Standard Form 298 (Rev.2-89)
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Yearly Progress Report for:
Rapid, Reagent-less Detection and Discrimination of Biological Warfare (BW) Agents using Multi-Photon, Multi-Wavelength Processes within Bio-Molecular Architectures

N. Scott Barker – University of Virginia

Reporting Period: 1 June, 2009 to 30 November, 2011

Grant #:W911NF-09-1-0270

Project Title: Terahertz Science & Technology: Submillimeter-wave Resonators for Investigation of the Dynamical Properties of Biological Molecules

Overall Project Goal: To create a sensitive permittivity measurement method for aqueous biological solutions. In order to take advantage of the high sensitivity of open-air resonators, accurate permittivity data of liquid references are to be obtained in order to overcome the difficulty in fully modeling open-air systems and thus allowing for smaller volumes and more elaborate setups to be used with a perturbation method.

Research Goals: 1) Accurately model a concentric liquid-tube-circular cavity resonator system in order to extract permittivity from measured resonant frequencies and Quality factors . 2) Determine system design for resonant modes with optimal sensitivity to polar liquids. 3) Scale resonator system for measurement at millimeter- and submillimeter-wave frequencies. 4) Measure liquids and extract permittivity.

Impact of the Research: To supplement the characterization of biological molecules by obtaining precise permittivity data for water and aqueous solutions at frequencies not obtainable by current spectroscopic methods.

Technology Transfers & Research Collaborations:

Merit of the Research: The creation of a liquid permittivity measurement system at lower terahertz frequencies that are not well-covered by traditional microwave and quasi-optical methods. This will entail creating a novel electromagnetic model that combines closed waveguide and free-space radiation, which would enhance the accuracy and possibilities of such cavity methods. Ultimately this research would examine the generalized use of a cavity resonator measurement system, which has until now been limited to specific types of modes.

Summary of Achievements: Tasks completed in the period include,

- Swept-frequency model of cavity and nested dielectrics
- Comparison of model to measurements

- each summary achievement listed above should have: (i) a title; (ii) a clear and concise body description; and, (iii) one or more illustrations (with captions), that clearly and concisely explains the importance of the achievement in the context of the program.

IMPORTANT NOTE #1: It is required that you attach a supplemental report that elaborates on and supports each of the individual achievements listed above. Each supplemental report should have a title page with the following at the top: **Supplement Report for "Achievement #1"** The information contained in this report could be a published paper, prior monthly report, viewgraph presentation, summary of important data, etc. There is no limit to what can be submitted for this part, but bear in mind that the subject should be presented so that it is easy to understand and in a manner that explains the general importance of the accomplishment in the context of the program.

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1 Project Overview

This project is concerned with the development of a precision measurement technique for determining the complex dielectric constant (or permittivity) of biological molecules at frequencies below 300 GHz. The development of precise measuring techniques is critical for advancing understanding of the interaction between biological molecules and terahertz (THz) frequency electromagnetic fields. Measurements obtained via quasi-optical systems such as THz Fourier transform spectroscopy and pulsed THz time-domain spectroscopy (TDS) have demonstrated spectra with repeatable features dependent upon the specific molecular structure of the sample being measured (e.g. hybridized vs. denatured DNA). Work has been done to transform transmission and reflection measurements into a refractive index and absorption coefficient, but the measurements are heavily subject to an intricate process of preparing the samples [1]. It is the absolute values of these measurements that provide values of the complex dielectric constant and therefore the precision is limited by the sample preparation. Precise values of the dielectric constant are needed in order to compare with and validate the data produced by theoretical models which can then be used to assign observed spectral features (vibrational modes) to specific structural features and topologies of the biological molecules. Additionally, these measurements have mostly been done with dry DNA; it is preferable to measure DNA in a liquid phase, in which it functions naturally [2]. Fourier transform spectroscopy measurements have been done with DNA in water, but the absolute value of transmission is not well reproducible.

Of particular interest is the measurement of biological molecules at mm-wave frequencies (60-300 GHz), where remote sensing of biological warfare is more promising [3]. However, most of this bandwidth falls at or below the minimum frequency of quasi-optical terahertz techniques. From the other end of the spectrum, broadband measurement techniques using waveguide exist, but the measurement uncertainty rises with increasing frequency. Instead, higher precision can inherently be obtained with a resonant system. Open-cavity resonators provide the best quality factors, ~100,000, but they require windows of samples volumes that are much larger than the beamwidth, and thus are not conducive to precise modeling of biological liquid samples. To circumvent this problem, the cavity perturbation technique can be used with open cavity resonators to allow for flexibility with sample size and containment, but calibration with a known standard is required. Unfortunately at these frequencies, few liquids have been measured, and the one most studied, water, is only known to within 5% precision or worse - this uncertainty places a lower limit on the possible precision of a permittivity measurement requiring calibration.

Waveguide cavities have been used to obtain the permittivity of liquids by measurement of the lowest order resonant mode, guaranteeing single-moded operation and thus ease of modeling from fundamental principles. However, due to cavity size scaling with frequency, measurements with the fundamental mode have been limited to below 50 GHz. Recent work has instead investigated the rigorous modeling of over-moded cavities [4]. By the ability to keep the cavity large and easily machineable, such an approach would enable the use of a resonator for acquisition of high precision measurements at higher frequencies. Additionally, a multi-moded cavity means that measurements can be taken at multiple frequencies, which is not the case for the single-moded approach; higher-order modes also offer higher quality factors. This is the method adopted by this project, and developed for the measurement of liquids. A preliminary measurement setup was created and tested, then used a guide for a new measurement setup. Concurrently the modeling was developed, starting from a closed resonator to the more accurate, yet complex, four-port junction.

2 Method and preliminary work

The measurement setup of an over-moded cylindrical cavity with an integrated fluidic setup is seen in Figure 1. In the center of the cavity is a hole, through which a low-loss quartz tube is inserted. A cylindrical cavity was chosen for its higher quality factors and symmetry with circular cross-sectional fluidic components, which facilitates modeling of the system. Fluidic samples are introduced into the cavity region by being pumped through the quartz tube with the aid of external fluidic components, as shown in Figure 2, which is a photograph of the preliminary setup. Measurements were taken with a vector network analyzer capable of 1 Hz frequency resolution; the resonances of the empty cavity can be seen in Figure 3, while measurements of various liquids can be seen in Figure 4.

In order to extract the permittivity from measurement, the modeling was developed in two stages. A general diagram showing the breakdown of the cavity setup relevant to modeling is shown in Figure 5. Since

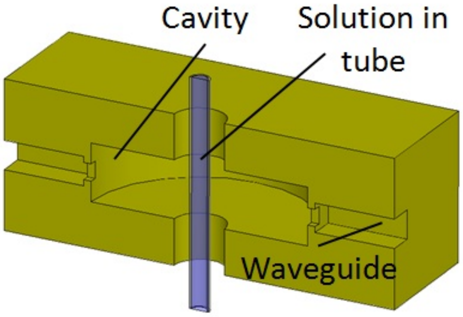

Figure 1: Diagram of tube placement within cavity.

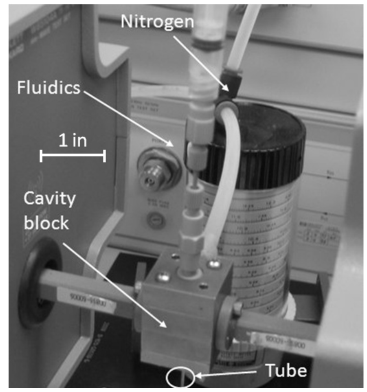

Figure 2: Complete Setup.

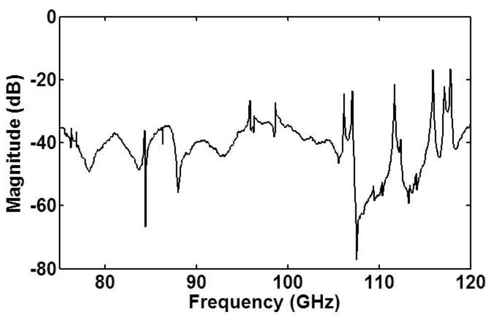

Figure 3: Measured S_{21} of the original cavity.

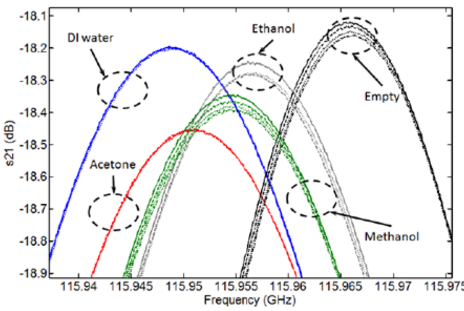

Figure 4: Preliminary measurements for the empty tube and four different liquids.

this cavity is mostly closed and of a simple geometry, the fields in each region can be approximated by a sum of discrete modes. The mode-matching technique is then applied, whereby the generalized scattering parameters are computed by satisfying the boundary conditions between dissimilar regions. With the first stage of the modeling, perfect electric walls were placed at ports 3 and 4, which was thought to be an acceptable boundary condition for measured high quality factor-modes, whose fields predominately remain near the cavity walls and away from the center. However, in the second, and current, stage, the full four-port structure is modeled.

For the first stage, the modeling was initially done in two separate parts in order to test its applicability and validity to the measurement problem. First, the setup was treated as a closed resonant system, containing only the nested dielectrics and the height discontinuity between the hole and the cavity; referring to the diagram of Figure 5, this included regions 1 to 4, with the aperture windows on the cavity region surface shorted with perfect electrical walls. However, it was found that this solution could not model the mode-mixing that occurs with over-moded cavities because there is no information of the coupling and thus the differing strengths of excitations of the various cylindrical cavity modes. This became apparent with the modeling of the waveguide-coupled empty cavity, i.e. regions 1-6, with regions 1 and 2 defined as air. Using the nominal dimensions of the preliminary cavity, the modeled S_{21} is shown in Figure 6, along with the electric field plot of the circled resonance in Figure 7, which shows the presence of two modes, the predominant TM910 mode but also the two center lobes of the TM140 mode. The strength of the TM140 mode relative to TM910 cannot be attained with the closed resonant model. This guided the pursuit of modeling the S-parameters of the cavity system.

Once the modeling of all of the regions was completed, it was examined with the interests of permittivity measurements. Since the modeling relies on setting an upper-limit to an infinite sum of modes, it is necessary to determine how many modes are needed until the varying solution settles to within an acceptable range, which is guided by the desired precision in the permittivity results and the measurement uncertainty. Examining convergence entails altering the number and types of modes that are summed, and compiling resonant

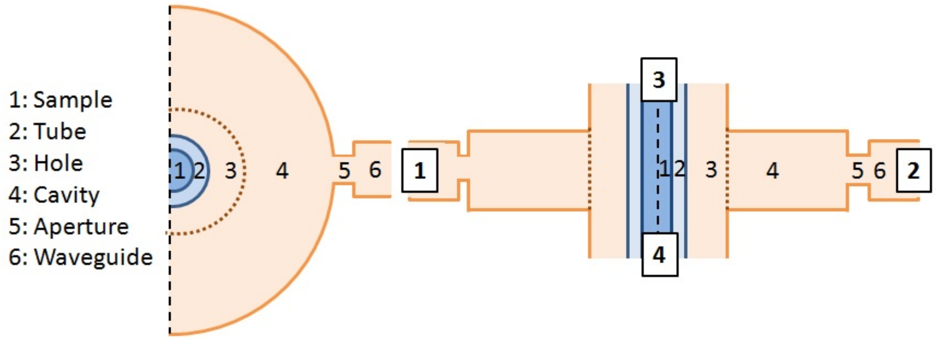

Figure 5: Cross-sectional views of regions (1-6) and port labels (1-4) for mode-matching analysis.

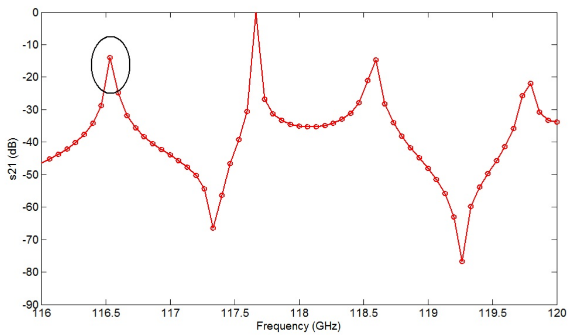

Figure 6: Modeled S_{21} of the empty cavity and hole regions, with aperture-coupled waveguides.

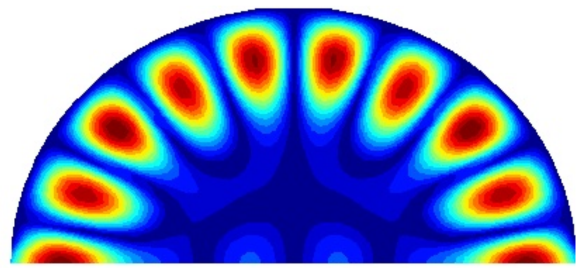

Figure 7: Electric field plot of circled 116.5 GHz mode.

frequency and quality factor data. There are varying ideas in the literature about what modes to choose and what sets the upper limit; generally a cutoff frequency is chosen, and the propagating modes within all the regions are summed, or the numbers of modes are set by the geometrical ratios of the discontinuities. However, if only certain types of modes are known to be excited, then other modes can be excluded from the simulation, which would free up computing resources. Modes are separated into three different indices that each correlate to a different coordinate in the 3D space. With this modeling, the number of modes in each region and along each direction was set by the geometrical ratio. For instance, looking at the geometry of the cavity in Figure 8, at the cavity-aperture discontinuity, the ϕ- and y-vectors were assumed to be nearly parallel. So, the number of modes along the y-direction in the aperture was chosen, and then the number of ϕ-modes in the cavity was scaled from the highest y-index, by the ratio of half the cavity circumference to the aperture width

Results from a few different methods of selecting modes within the aperture are shown in Figure 9; the resonant frequency is plotted against the number of ϕ-modes within the cavity. The red and blue curves resulted from choosing all aperture modes that propagate under a cutoff frequency that is higher than the maximum frequency of interest. The difference between the two is that for the blue curve only up to 20 cavity modal indices in the axial direction (x-modes) were used, whereas the red curve used the full amount. As the two are nearly indistinguishable, this suggests that higher order x-modes can be neglected. It can be seen that the resonant frequency has converged to within 600 kHz, and with more modes this could decrease further. This convergence is approaching the measurement uncertainties ranging around 300 kHz of the data seen in Figure 4 and is certainly smaller than the MHz-order differences in the resonant frequencies among the liquids.

The modeling was also initially compared with measurements, first those of the empty cavity and the cavity containing an empty quartz tube. The cavity radius (a difficult dimension to measure) was tuned so that the model resonant frequency matches that of the measurement. Then, using its nominal dimensions, the quartz tube is added; the results and comparison to data can be seen in Figure 10. It was found that the

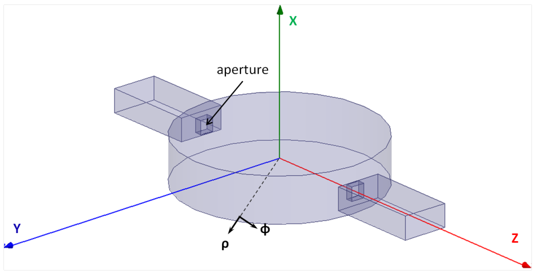

Figure 8: Setup of coordinate system for modeling of cavity.

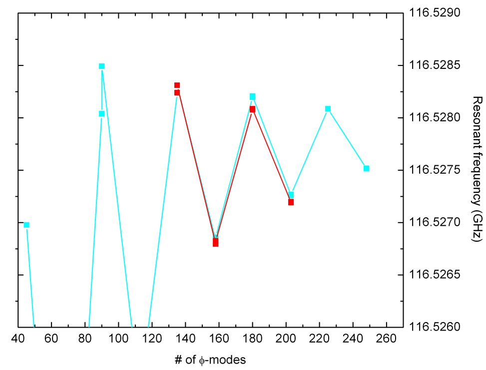

Figure 9: Resonant frequency convergence to below 600 kHz for two different methods of mode selection.

modeling could capture the increase in resonant frequency with tube insertion, which also points to complex mode-mixing effects that occur with over-moded cavities; for an isolated single-mode, the resonant frequency should decrease with the addition of dielectrics.

The effect of finite conductivity of the cavity walls was also investigated, as the results shown in Figure 10 demonstrated significant differences between the quality factors and S_{21} magnitudes of the measurement and model. Work began on including conductive loss in the cavity walls; an initial result for the resonance that has been measured can be seen in Figure 11. The resonance broadened, indicating a lower quality factor. However, when the simulation was extended to a broader frequency range, erroneous results ensued near 118 GHz, shown in Figure 12 - there was a severe dip that is not otherwise seen in the measurements or in equivalent HFSS simulations. This was further investigated, and as a result, a discontinuity problem was discovered with the equations. It had not previously been seen due to its narrow bandwidth but became apparent when the frequency range was reduced to 20 Hz. Based on simulations of differing cavity dimensions and electric-field plots, it was believed to occur at a cutoff frequency for a mode that is important for aperture-to-cavity coupling. We were not sure what is causing this dip to occur; while the problem seems to be related to a division by zero factor, the complexification of the wavenumber should, in theory, resolve this issue. It was thought that perhaps the small-angle and fields approximation taken at the cavity-aperture interface omits fields that would subdue the effects of this mode, so a numerical integration was performed that included components of the longitudinal aperture field that would be tangential on the circular interface. However, this erroneous dip remains, although its behavior is altered.

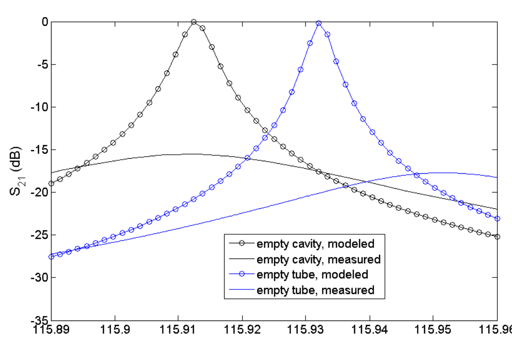

Figure 10: Modeling and measurement of impact on resonance due to tube insertion.

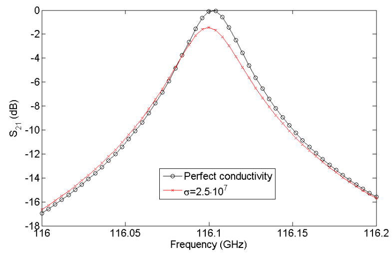

Figure 11: Effect of cavity wall loss on resonance of interest.

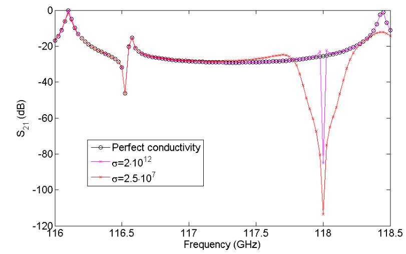

Figure 12: Broadband results of effect of cavity wall loss of various conductivities.

3 Current status

The second stage of the custom modeling of the cavity is close to completion. With shorting ports 3 and 4, there was concern for the effects of reflection from possible wave propagation up the insertion hole, which would be exacerbated when dielectrics are introduced because they would lower the cutoff frequency for propagation through the hole. Thus for improved accuracy, the modeling of the cavity was reformulated so that the aperture, cavity, and insertion hole are modeled as a four-port junction, allowing for any arbitrary termination of the hole. The main difference is the addition of circular waveguide modes to the cavity and material regions, which previously only contained standing waves. For modeling of the inner dielectrics, the inclusion of circular waveguide modes necessitates a complex root finder that will solve for the necessary propagation constants; this has been completed and is currently being implemented in the modeling.

The cavity block used in the preliminary setup was not well-machined and thus difficult to model accurately. Using the nominal dimensions of the old cavity, a new block was designed and machined, though it was decided to rotate the waveguides so that predominately TE-cavity modes were excited; this was done to reduce the loss from the split in the block that is required from the limitations of machining. Additionally, in order to reduce mode-mixing and contain modes with stronger center fields, the hole radius was reduced to that of the quartz tube.

The environmental controls were also improved, as to reduce the uncertainties seen in the preliminary data. At the time, there was no control of the temperature, and only some purging of the cavity air. With the new modeling, the impact of the measurement environment was investigated. Previously, the temperature could only be characterized with a thermometer with 0.1°C precision, which for an aluminium block translates to a change in dimension of 2.3 ppm; applying this to the cavity radius results in a frequency shift seen in Figure 13, a change of about 500 kHz, which would limit the precision at which the permittivity could be determined. Likewise, the impact of relative humidity was examined, and the resulting 6 MHz shift seen in Figure 14 is on the order of the previously measured data.

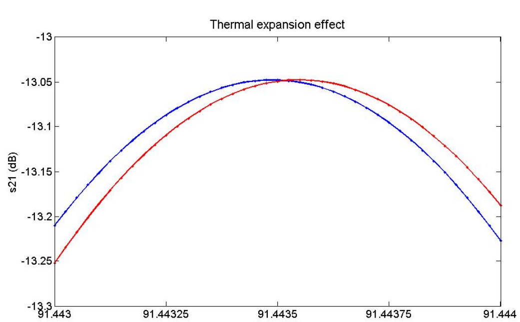

Figure 13: Thermal expansion effect on resonant frequency with 0.1°C temperature uncertainty.

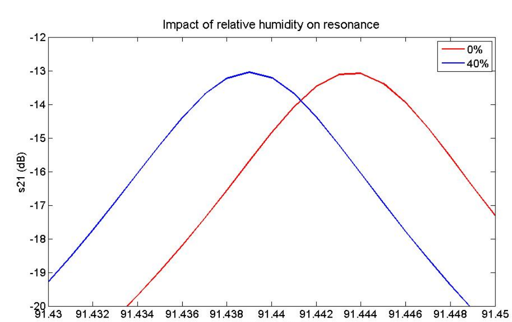

Figure 14: Impact of relative humidity of cavity on resonant frequency.

Solutions of these effects were incorporated into the final measurement setup shown in Figure 15. The cavity block contains the cylindrical cavity and also a concentric insertion hole for the quartz tube that holds the test liquid for measurement. At the top of the block the insertion hole expands in order to hold the fluidic fitting that interfaces the quartz tube to a syringe; additionally there is a #8-32 threaded hole that will accept a bolt mount thermistor sensor for the monitoring and feedback control of the cavity temperature. Consequently the sides of the cavity block were modified for the symmetrical mounting of two heating elements; with this arrangement of heaters and sensor, it is believed that the temperature of the cavity and liquid can be maintained to within less than 0.1°C. Surrounding the remaining sides of the cavity are waveguide line sections, or nitrogen blocks, whose purpose is to provide inlet and outlet holes for nitrogen gas to flow through the cavity and prevent excess sample and water vapor from entering the cavity; a hole runs from the tube adapter to the top wall of the waveguide, as Figure 16 shows. The waveguides will be plugged with epoxy so that the nitrogen will enter the cavity and not escape in the opposite direction into the external network analyzer equipment. These nitrogen blocks will be included during network analyzer calibration in order to remove loss from the waveguide and the epoxy.

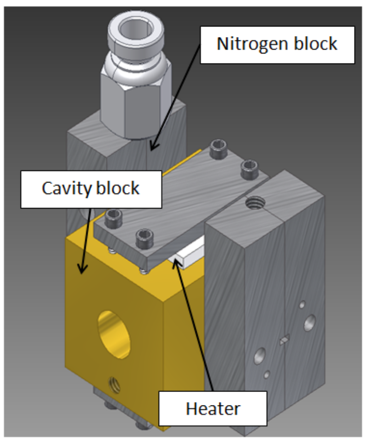

Figure 15: CAD of new measurement setup.

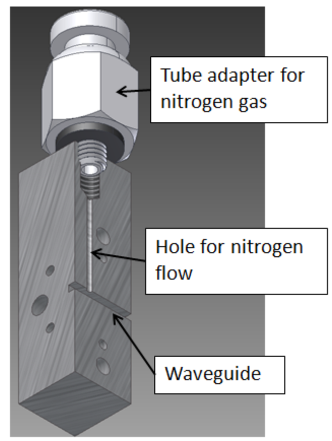

Figure 16: CAD of one half of nitrogen block.

All of the parts have been machined, and currently the environmental controls are being developed. The new cavity was measured, and there is good agreement with the modeling, as seen in Figure 17. This shows the validity of the model, and with the inclusion of complex root finder for the dielectrics, it will be possible to back out the permittivity from measured data. The tight environmental controls placed on the measurements should produce more precise permittivity data of liquid standards, in aid of more precise characterization of liquid biological samples at frequencies not attainable with the quasi-optical methods.

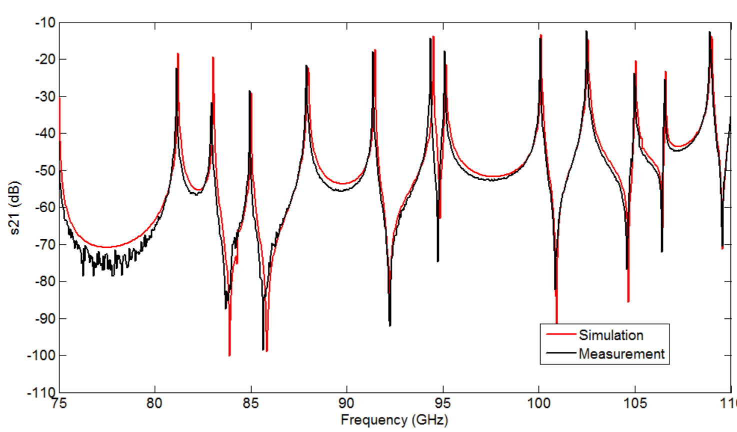

Figure 17: Comparison of measurement and modeling of empty cavity.

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Presentations at Conference or other Relevant Technical Meetings

- oral presentation at 2009 Nanoelectronic Devices for Defense & Security

Honors and Awards

- Best Student Presentation Award, 2009 Nanoelectronic Devices for Defense & Security Conference

Researchers Supported

- Angelique Sklavounos, graduate student – 100%